X-ray Study of Anti-phase Boundaries in Quadruple-period Ordered $GaAs_{0.87}Sb_{0.13}$ Alloy Films

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Introduction: Anti-phase domain boundaries (APB) are important structures in atomically ordered materials. Recent studies have shown that the APBs can affect the electronic properties of the material, such as carrier mobility. In this work, we extend the earlier study of APBs in bulk ordered metallic alloys by Warren[1] to ordered thin films. A three dimensional structural model has been proposed to explain the diffraction phenomenon of APBs.

Methods and Materials: We used a quadruple-period ordered $GaAs_{0.87}Sb_{0.13}$ as a sample. X-ray diffraction was performed on a four-circle diffractometer with an x-ray energy of 8.048 keV.

Results: The upper panel of Fig. 1 shows a measured large area x-ray reciprocal-space-map. Quadruple-period ordering peaks were observed at lateral positions 1.25, 1.75, 2.25,and 2.75 in (002) and (003) reciprocal lattice planes. It is interesting to note that the peaks are quite narrow in the lateral direction. However, they are stretched along [001] direction forming weak streaks running all the way from (hk2) to (hk3) planes. This indicates that the coherent length in the [001] direction is small.

Considering that our structure is atomically ordered and that anti-phase domain boundaries are the major defects, we therefore consider a structural model with statistically distributed anti-phase domains, and assume that these domains have independent position and size distributions along the crystallographic axes [110], [-110] and the [001]. Thus the diffraction intensity can be written as, after Warren,

$$I(\mathbf{q}) = \left| \sum_{m1,m2,m3} F(\mathbf{q}) \exp(2\pi i \cdot \Phi(m1, m2, m3)) \cdot \exp(2\pi i \mathbf{q} \cdot (m1 \cdot \mathbf{a} + m2 \cdot \mathbf{b} + m3 \cdot \mathbf{c})) \right|^2$$

Where, $\Phi(m1,m2,m3)$ is the phase factor related to the transition of one domain to another. (**a**,**b**,**c**) are the unit vectors of the [110],[-110], and [001] axes, resp. $F(\mathbf{q})$ is the structure factor of the ordered super cell. By carefully considering the distributions of the APBs, we can fit the measured data theoretically. The lower panel of Fig. 1 shows the best fit to the measured reciprocal space map, which yields average domain sizes along the unit cell axes [110], [-110], and [001] to be 130, 400, and 5 nm, respectively, for our particular sample. The small domain size in the [001] direction explains quite well the [001] streaks in the reciprocal space map.

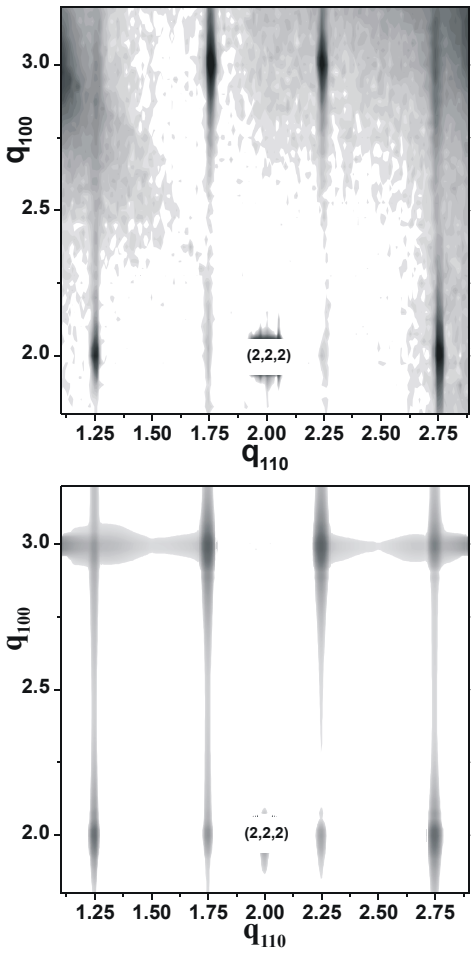

Figure 1. X-ray reciprocal space maps in the (-110) plane. Experimental and simulation results are shown in the upper and lower panels, respectively.

Conclusions: Based on a structural model containing random distribution of APBs in quadruple-period ordered thin film, we explained successfully the diffraction pattern with long streaks running along [001] direction in the reciprocal space map. The information of APBs will help us to understand better the ordering phenomena as well as the difference in the lateral widths seen in our [110] line scans.

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References: 1. B.E. Warren, X-ray diffraction, (Dover, New York,1990).